Metabolic Modelling, Spring 2009, Exercises
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Solutions

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1. Building the stoichiometric matrices.

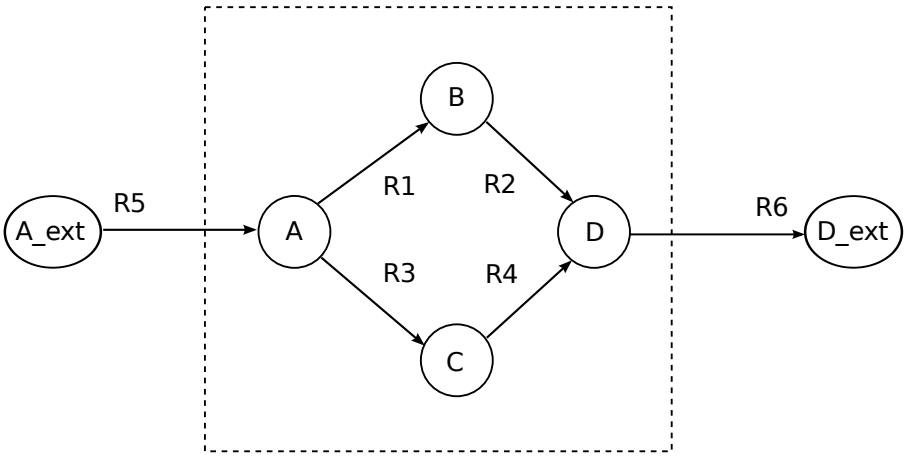

Figure 1: Substrate graph of the system with inner/outer boundary.

```
>> Stot

Stot =

     0    -1    -1     0  |   1     0
    -1     1     0     0  |   0     0
     0     0     1    -1  |   0     0
     1     0     0     1  |   0    -1
  ------------------------+----------
     0     0     0     0  |  -1     0
     0     0     0     0  |   0     1

>> Sexc

Sexc =

     0    -1    -1     0     1     0
    -1     1     0     0     0     0
```

```
     0     0     1    -1     0     0
     1     0     0     1     0    -1
```

2. Flux vectors

```
>> v1

v1 =

     0
     0
     1
     1
     1
     1

>> v2

v2 =

     1
     1
     0
     0
     1
     1

>> S*v1

ans =

     0
     0
     0
     0

>> S*v2

ans =

     0
     0
     0
     0

>> S*[0  0  0  0  0  0]'

ans =

     0
```

```
       0
       0
       0

>> S*(v1+v2)

ans =

       0
       0
       0
       0

>> S*(v1+1)

ans =

      -1
       0
       0
       1

>> S*(v1-2*v2)

ans =

       0
       0
       0
       0
```

Valid flux vectors produce zero-vector when multiplied with S. Thus, $v_1 + 1$ is not a valid flux vector.

3. Null spaces

```
>> Kexc = null(Sexc)

Kexc =

   -0.5393    0.2062
   -0.5393    0.2062
    0.4482    0.3639
    0.4482    0.3639
   -0.0910    0.5701
   -0.0910    0.5701

>> Ktot = null(Stot)

Ktot =
```

$$
\begin{bmatrix}
-0.5000 \\
-0.5000 \\
0.5000 \\
0.5000 \\
-0.0000 \\
0.0000
\end{bmatrix}
$$

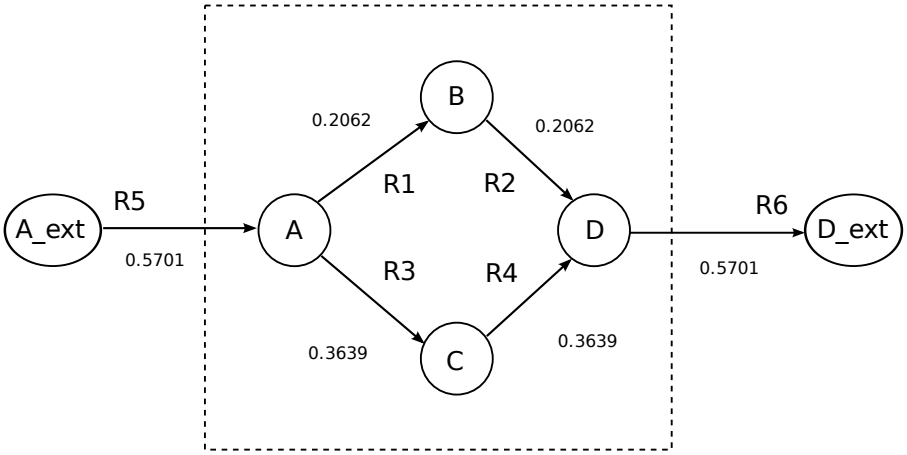

Figure 2: First basis vector of the exchange kernel matrix used as the fluxes.

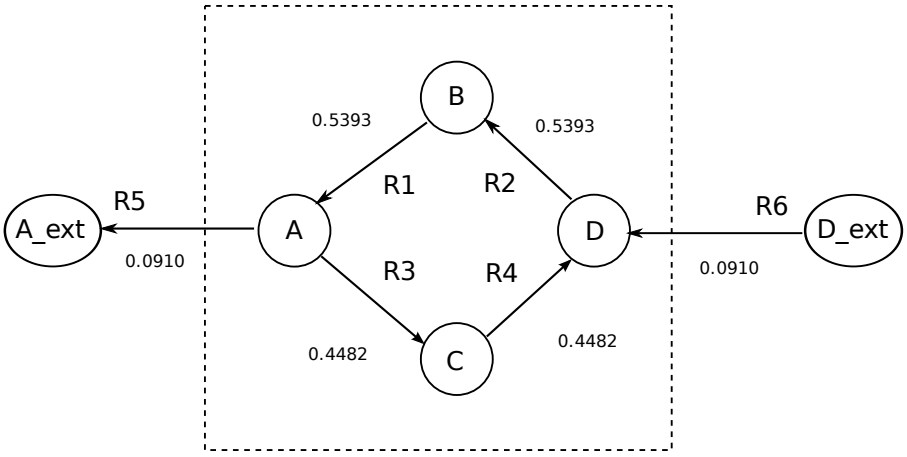

Figure 3: Second basis vector of the exchange kernel matrix used as the fluxes.

With total stoichiometric matrix, reactions 5 and 6 can't operate in steady state. By definition, in steady state the out-flux and the in-flux of a metabolite have to be equal. Thus, A_{ext} and D_{ext} can't have any flux as they are not produced/consumed.

4. Kernel matrices.

   Enzyme subsets are defined as those reactions of the system, whose rows have fixed ratio in the kernel matrix of the system. For K_{exc}, it's easy to

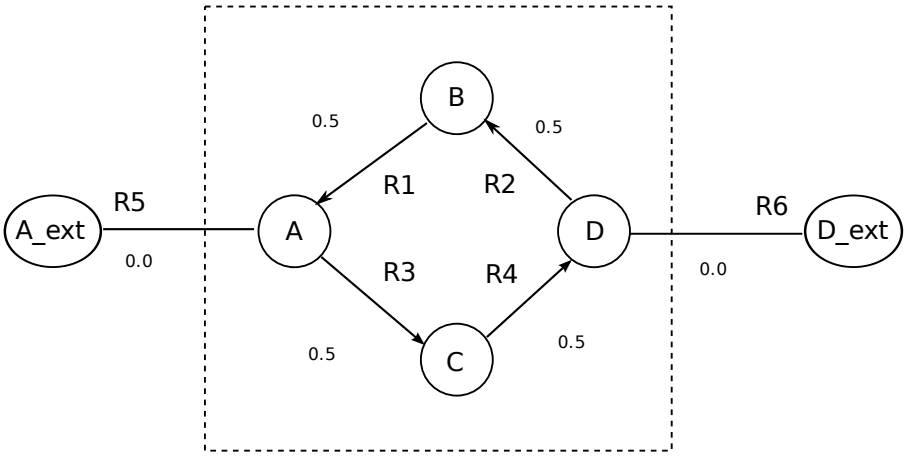

Figure 4: The sole basis vector of the total kernel matrix used as the fluxes.

see that reactions {1,2}, {3,4}, {5,6} form the enzyme subsets.

For K_{tot}, from the definition of enzyme subsets, all the reactions form an enzyme subset. This is bit misleading though, as reactions 5 and 6 are zeros, and thus can't operate in steady state. Thus more meaningful would be to state that only reactions 1,2,3,4 are in enzyme subset. The whole question about enzyme subsets with only one basis vector is questionable anyway: for a single vector, any two rows always have a fixed ratio between them. The question about enzyme subsets is thus not really meaningful with $n = 1$ dimension kernel matrices.